Are the high-T_c superconductors strongly correlated electron systems?

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In this paper, we argue that the high-temperature superconductors do not belong to strong correlated electron systems. It is shown that both the two-dimensional Hubbard and t-J models are inadequate for describing high temperature superconductivity. In our opinion, a superconducting phase should be an energy minimum electronic state which can be described in a new framework where the electron-electron interactions (both on-site Hubbard term and off-site term) and the electron-phonon interaction can be completely suppressed.

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The mechanism of high temperature superconductivity, despite great efforts from both theoretical and experimental approaches since 1986[1], remains an almost complete mystery in condensed matter physics. As is well known, the undoped parent compounds of the high temperature superconductors are so-called Mott insulators and the superconductivity can be achieved by doping carriers into these materials. It is widely believed in the physical community that a comprehensive understanding of the doping evolution from insulating to superconducting state may help to uncover the underlying mechanisms of high temperature superconductivity. However, although under intensive studies for about twenty-five years, physicists do not agree on how superconductivity works in these materials.

Theoretically, it is generally accepted that the conventional superconductors are well-described by the BCS pairing theory of the electron-phonon interaction mechanism[2], while the high-temperature superconductors are strongly correlated electron systems that may need a new (or at least improved) theory. Many researchers blindly believe that the Hubbard[3] and t-J models[4] can capture the essential physics of the high-temperature superconducting phenomenon. Thousands of articles based on these two models have been published during the past several decades. Unfortunately, no one of these works is now known to be a valid interpretation of the phenomena in cuprate superconductors. We think that in such a situation researchers should consider some fundamental issues of high-temperature superconductivity, for example, do the high-temperature superconductors belong to strong correlated electron systems? Are the Hubbard and t-J models valid to be used to describe the superconductivity?

In this paper, we argue that the old theoretical framework of the superconductivity has an unrecognized flaw. Based on the energy minimum principle and the experimental observation of quasi-one-dimensional charge stripes[5], a new framework is proposed to describe all superconductors.

Let's start with a very basic question: What causes the resistance in the metal materials? In the framework of classical physics, a metal consists of a lattice of positive ions surrounded by a sea of electrons that will drift from one end of the metal to the other under the influence of an applied electric field. During this procedure, the electrons will lose some of their kinetic energy due to the scattering by the thermal motion of ions or collision with other electrons, as shown in Fig. 1, which are the two main source of resistance. Obviously, when a material is driven into the superconducting state, the superconducting electrons will no longer be scattered by the ions, and the electron-electron collisions are also completely eliminated in the superconductor.

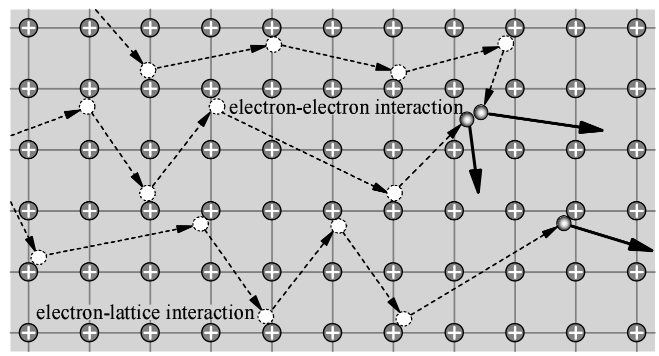

Figure 1: In classical physics, the resistance mechanism consists of two parts: the main part is contributed by the electron-lattice interactions (scattering), another part is a result of electron-electron interactions (collision), as illustrated in this figure. In our opinion, the most important question concerning the mechanism of superconductivity will be converted into a simple question: how can these two kinds of interactions be avoided when the material goes into the superconducting state?

To be a reliable theory of superconductivity, it must provide a clear description or explanation of how the two kinds of interactions (see Fig. 1) can be fully suppressed when a superconductor goes from the normal state into the superconducting state. Unfortunately, almost all existing theories of superconductivity have neglected these

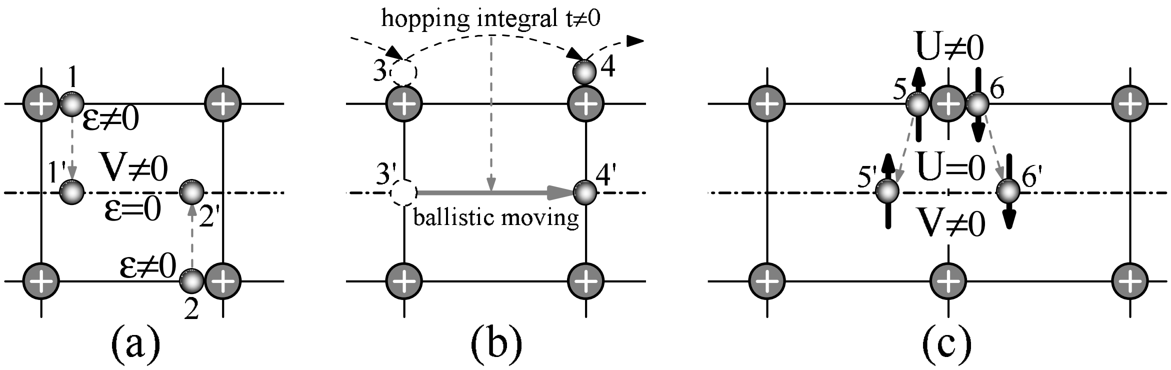

Figure 2: The explanation of why the three physical parameters (on-site energy ε, hopping interaction t and the strong Hubbard interaction U) given in Hamiltonian form in second-quantization theory are invalid to be used for describing the phenomenon of superconductivity. (a) The on-site energy ε, (b) hopping interaction t, and (c) the Hubbard interaction U, they can very easily be excluded from the Hamiltonian if electrons are located in the equilibrium positions (1' , 2', 3', 4', 5' and 6') of zero potential energy.

basic physical facts. So far, the researchers in the field of superconductivity are used to do their calculations by blindly applying the Hamiltonian handed down from generation to generation, physically, it is most likely that they are on the wrong track. Note that the complex numerical simulations cannot generate any results that are not already implied in the framework. In our opinion, the reason why the mechanism of high temperature superconductivity still remains unknown lies in the fact that the key factors of Fig. 1 are not considered in the Hubbard and t-J models.

The Hubbard model is the simplest model of interacting particles in a lattice, which is mathematically defined by following Hamiltonian

$$H = -t \sum_{\langle ij \rangle \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where t is the hopping matrix element between the nearest neighbor sites of the lattice, U is the on-site Coulomb repulsion, $c_{i\sigma}$ ($c^{\dagger}_{i\sigma}$) annihilates (creates) an electron with spin σ at site i, and $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$.

In 1977, Jozef Spalek derived the so-called t-J model from the above Hubbard model. The corresponding Hamiltonian also consists of two pieces:

$$\begin{aligned} H &= -t \sum_{\langle ij \rangle \sigma} \left[c^{\dagger}_{i\sigma} (1 - n_{i-\sigma})(1 - n_{j-\sigma}) c_{j\sigma} + H.c. \right] \\ &\quad + J \sum_{\langle ij \rangle} (S_i S_j - \frac{1}{4} n_i n_j). \end{aligned} \quad (2)$$

where t is an effective transfer integral, J ($= 4t^2/U$) is the antiferromagnetic exchange energy for a pair of nearest neighbor sites $\langle ij \rangle$, S_i and S_j are spin-1/2 operators.

Do the Hubbard and t-J models capture the key physics of the high-temperature superconductivity?

From the energy point of view, a stable superconducting state must first be an energy minimum electron coherent state with the complete suppression of the electron-electron and electron-ion interactions inside the superconductor. However, the theoretical frameworks of Hubbard and t-J models apparently overlook these factors.

According to the Hamiltonian of Eq. (1), if two electrons are on the same site (with oppositely directed spin), the second term will be extremely large because of strong on-site Coulomb repulsion. Although this hypothesis does not violate the Pauli exclusion principle, the configuration with two electrons of opposite spin on the same site is harmful to the formation of the superconducting state. Hence, the second term of Eq. (1) must be ruled out. Without the contribution of the second term, the Hubbard model will automatically change into the conventional tight binding model from regular band theory. Of course, the retained first term of Eq. (1) is also impossible to describe the superconducting behavior, since the hopping picture is in fact an idealized model of electron-ion interactions (scattering) as shown in Fig. 1. In other words, both the two terms of the Hubbard Hamiltonian are contrary to the basic assumption of superconductivity that the electron-electron and electron-ion interactions should be completely eliminated. We expect that all the above discussions are also suitable for the t-J model of Eq. (2).

Obviously, the Hubbard and t-J models based on the Hamiltonian cannot be applied to explain superconductivity. In the following, we will discuss how to establish a correct theory of superconductivity. In the Wannier representation, the Hamiltonian can generally be decomposed into three parts, as shown in Fig. 2. The first part is the so-called on-site energy ε which originates from the strong short-range attraction between electron and ions, as marked by 1 and 2 in Fig. 2(a). This strong interaction ($\varepsilon \neq 0$) can be converted quite easily to the weak long-

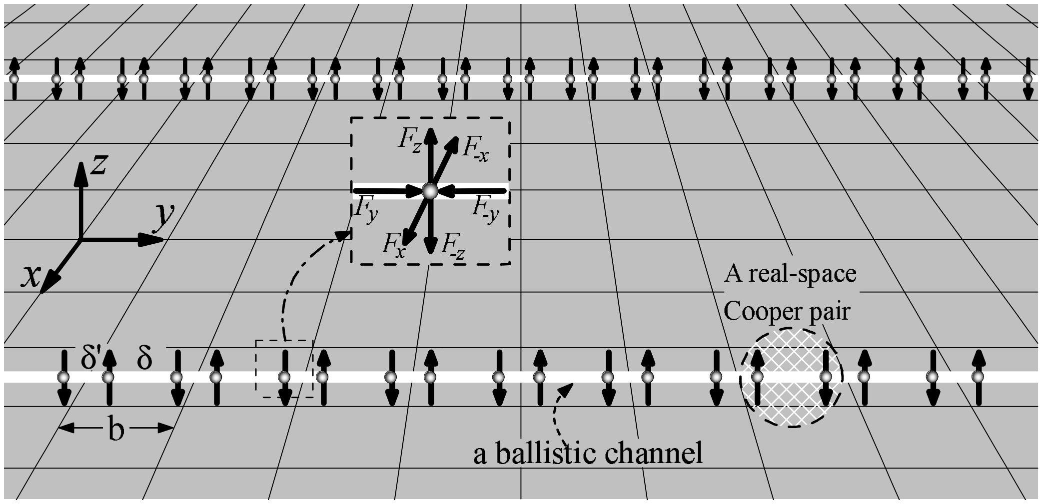

Figure 3: A real-space superconducting ground state where the charge carriers (electrons) can self-assemble into some static one-dimensional peierls charge and spin antiferromagnetic stripes. In this special case, it is easy to prove that the resultant force applied to each electron is equal to zero along any directions ($|F_x| = |F_{-x}|$, $|F_y| = |F_{-y}|$ and $|F_z| = |F_{-z}|$). In other words, the strong electron-electron Coulomb interactions within the stripe can be completely suppressed under this simple framework ($|F_y| = |F_{-y}|$) . Under the influence of the external fields, the peierls chains will transfer into periodic chains and the superconducting current can flow without resistance along the ballistic channels.

range electron-electron interaction ($V \neq 0$, $\varepsilon = 0$), if the two electrons are located in the equilibrium positions [1' and 2' in Fig. 2(a)] of zero potential energy. The second part is the hopping interaction t which is an extremely simplified picture (without involving any detailed hopping mechanism) of kinetic electron-ion interaction [from 3 to 4 in Fig. 2(b)]. As discussed above, the hopping picture is unsuitable to describe the phenomenon of the superconductivity. A more reasonable picture is to assume that the electron can tunnel from 3' to 4' through a ballistic channel, as also shown in Fig. 2(b). The third part is the strong on-site electron repulsive interaction (5 and 6 in Fig. 2(c) with Hubbard $U \neq 0$) which can also be easily avoided if the two electrons are assumed to be arranged in the equilibrium positions 5' and 6', as also shown in Fig. 2(c). In this case, the strong Hubbard interaction (elephant U) is replaced by a "soft" electron-electron interaction (mouse V).

Based on the minimum energy principle, all the charge carriers have the tendency to stay around the equilibrium positions with only the long-range (compared to the on-site Hubbard interaction) electron-electron Coulomb repulsion $V \neq 0$. Hence, the microscopic mechanism of the high-temperature superconductivity turns out to be a very simple problem: How can the repulsive interaction V between electrons be overcome in favor of the superconductivity? Obviously, the strong direct Coulomb repulsion between electrons cannot be suppressed by exchanging a small "second-order" quasiparticle, for example, the quantized phonon induced by the lattice vibration. In fact, the strongly repulsive electrons can be "glued" together purely by a real-space electronic mechanism.

The determination of the superconducting ground state is the key theoretical issue in the study of the mechanism of the superconductivity. What is the superconducting ground state and how to describe it? In the previous series papers[6–12], it has been elucidated that the formation of the quasi-one-dimensional charge stripes in the superconductors plays the fundamental role of the superconductivity. In our approach, the most basic unit of the superconducting ground state is the static one-dimensional peierls charge and spin antiferromagnetic chain[7], as shown in Fig. 3. It has been proven analytically that without applying the external field, the charge carriers (electrons) can self-organize into some one-dimensional peierls charge chains with $\delta + \delta' = b$ (see Fig. 3), where b is the lattice constant in the stripe direction. In this situation, the resultant force applied to each electron is exactly zero along any directions ($|F_x| = |F_{-x}|$, $|F_y| = |F_{-y}|$ and $|F_z| = |F_{-z}|$) . Moreover, a stable real-space Cooper pair can be defined inside one plaquette, as also shown in Fig. 3.

Under the influence of the external fields, the transition from the ground state into the excited state will occur for the superconducting electrons. Consequently, the peierls chains will transfer into some real-space periodic charge stripes with a definite electron-electron spacing of $\delta = b/2$. For an excited superconducting state, all electrons are identical and the electron-electron Coulomb repulsions can be naturally suppressed due to the symmetry of the real-space charge stripes. In this case, all the superconducting electrons will be condensed into a coherent state and the concept of Cooper pair will no longer has any physical meaning. In this scenario, the supercon-

ducting current can flow without resistance along many ballistic channels, as shown in Fig. 3.

Finally, we present a brief discuss about the validity of the BCS pairing theory. Recently, Hirsch argued that it is time to question the validity of the BCS theory of superconductivity[13]. Although we don't completely agree with all of his views, some of his arguments are physically reasonable and interesting. In our viewpoint, the pairing and superconductivity are two different and unrelated physical phenomena. The electron pairing is an effect of the short-range electron correlation, while the superconductivity comes from the long-range electron correlation (as shown in Fig.3). In fact, the pairing mechanism cannot effectively inhibit the generation of the resistance in the superconductor. Let us look at Fig. 1 again, the electron-lattice (or pair-lattice) interactions are avoidable even if all electrons are paired. In addition, the much stronger pair-pair Coulomb repulsion will inevitably lead to the generation of resistance. In our opinion, it is most likely that there exists some flaws in the electron-phonon interaction based BCS theory[14].

In this short letter, it has been pointed out that the high-temperature superconductivity has nothing to do with the strong correlated electron systems. It should be emphasized that any kind of materials materials will no longer be the strongly correlated systems when the materials enter into the superconducting states. We have shown clearly that both the Hubbard and t-J models are unsuitable to describe the high temperature superconductivity. It has been stressed that a reliable theory of superconductivity should be based on the energy minimum principle and both the electron-electron (on-site and off-site) and electron-ion interactions must be effectively suppressed. We have outlined a new theory of superconductivity proposed to apply to all superconductors (both conventional and unconventional).

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